Solutions to the time-dependent Schrodinger equation in the continuous spectrum case

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Abstract

We generalize the Lewis-Riesenfeld technique of solving the time-dependent Schrodinger equation to cases where the invariant has continuous eigenvalues. An explicit formula for a generalized Lewis-Riesenfeld phase is derived in terms of the eigenstates of the invariant. As an illustration the generalized phase is calculated for a particle in a time-dependent linear potential.

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The study of time dependent quantum systems has attracted considerable interest in the litterature. The origin of this development was no doubt the discovery of an exact invariant by Lewis and Riesenfeld [1] . The work of Lewis and Riesenfeld and others assumes that the eigenvalue spectrum for the invariant I is discrete. Let us recall that the general method to introduce the Lewis and Riesenfeld theory, valid whatever the time dependence of the parameters, considers invariant operators. For a system specified by a time-dependent Hamiltonian $H\left(\vec{X}(t)\right)$, and a corresponding evolution operator $U(t)$, an invariant is an operator $I(t)$ such that

$$\frac{dI}{dt} = \frac{\partial I}{\partial t} + \frac{1}{i\hbar}[I,H] = 0. \tag{1}$$

or

$$I(t) = U(t)\, I(0)\, U^{-1}(t). \tag{2}$$

It possesses a remarkable property that any eigenstate of $I(0)$ evolves into an eigenstate of $I(t)$. Then, if the set of reference eigenstates $\{|\phi_n(t)\rangle\}$ for the operator $I(t)$ are continuous with respect to t (all eigensates are associated with the same time-independent eigenvalue ε_n), the corresponding global phases $\theta_n(t)$ are defined by the relation associated to the wave functions $|\psi_n(t)\rangle$:

$$|\psi_n(t)\rangle = U(t)\mid\phi_n(0)\rangle = e^{i\theta_n(t)}\mid\phi_n(t)\rangle. \tag{3}$$

It follows from the Schrödinger equation for $|\psi_n(t)\rangle$

$$i\hbar\frac{\partial}{\partial t}|\psi_n(t)\rangle = H(t)\psi_n(t)\,|\psi_n(t)\rangle\,, \tag{4}$$

that $\theta_n(t)$ satisfies the relation

$$\hbar\frac{d}{dt}\theta_n(t) = \langle\phi_n(t)\mid i\hbar\frac{\partial}{\partial t} - H\mid\phi_n(t)\rangle. \tag{5}$$

One way to describe the exact quantum evolution of Lewis and Riesenfeld is to introduce the concept of elementary projectors on an eigenstate $|\phi_n(t)\rangle$ of the invariant operator $I(t)$

$$P_n(t) = \mid\phi_n(t)\rangle\langle\phi_n(t)\mid. \tag{6}$$

It is easy to verify that each projector $P_n(t)$ is therefore a constant of the motion i.e., $P_n(t) = U(t)\, P_n(0)\, U^{+}(t)$.

We can state that the exact evolution described by equations (3) and (5) can be formally written in the following form

$$\forall t: \ U(t) P_n(0) = P_n(t) U(t). \tag{7}$$

Notice that if, initially, the system is in the eigenstate $|\phi_n(0)\rangle$ so that $I(0)|\phi_n(0)\rangle = \varepsilon_n |\phi_n(0)\rangle$, then $P_n(0)|\phi_n(0)\rangle = |\phi_n(0)\rangle$ and (7) gives

$$U(t)|\phi_n(0)\rangle = P_n(t) U(t)|\phi_n(0)\rangle. \tag{8}$$

In general the spectrum of I possess both discret and continuous eigenvalues. The Lewis and Riesenfeld theory in a continuous spectrum was raised for the first time by Hartley and Ray [2] where they extend the Lewis and Riesenfeld theory for a general Ermakov system to the continuous spectra like an anstaz and looks at the eigenfunctions in a continuous spectrum $|\phi(k;t)\rangle$ of the invariant operator $I(t)$ and the solution $|\psi(k,t)\rangle$of the Schrodinger equation in the form $e^{i\theta_k(t)}|\phi(k;t)\rangle$ .The limitation of the Hartley-Ray approach [2] is that, in general, there is no explicit formula of Lewis and Riesenfeld phase. Later Gao et al [3] calculate the Schrödinger solutions for a continuous spectrum using the path integral technique. In some papers [3] [4] the overall phase factor $\theta_k(t)$, interpreted in the spirit of the original investigation of Lewis and Riesenfeld, is actually obtained through the relation $\hbar\frac{d}{dt}\theta_k(t) = \langle\phi(k;t) \mid i\hbar\frac{\partial}{\partial t} - H \mid \phi(k;t)\rangle$.This procedure clearly parallel to that for the discrete spectrum is not founded. The reason is that the calculation of the expectation value $(i\hbar\frac{\partial}{\partial t} - H)$ with respect to the eigenfunctions $|\phi(k;t)\rangle$ analyzed trough examples in [4] lead to errenous results.

In the case of continuous spectrum we cannot numerate eigenvalues and eigenfunctions, they are characterised by the value of the physical quantity in the corresponding state. Althoug the eigenfunctions $|\phi(k;t)\rangle$of the invariant operators with continuous spectra cannot be normalised in the usual manner as is done for the functions of discret spectra, one can construct with the $|\phi(k;t)\rangle$ new quantities - theWeyl's *eigendifferentials (wave packets)*- [5] [6] which possess the properties of the eigenfunction of discrete spectrum. The eigendifferentials are defined by the equation

$$|\delta\phi(k;t)\rangle = \int_k^{k+\delta k} |\phi(k';t)\rangle\, dk'. \tag{9}$$

They divide up the continuous spectrum of the eigenvalues into finite but sufficiently small discrete regions of size δk .

The eigendifferential (9) is a special wave packet which has only a finite extension in space; hence, it vanishes at infinity and therefore can be seen in analogy to bound states. Furthermore, because the $\delta\varphi$ have finite spatial extension, they can be normalized. Then in the limit $\delta k \to 0$, a meaningful normalization of the function φ themselves follows: the normalization on δ functions.

For δk, a small connected range of value of the parameter k (this corresponds to a group of "neighboring" states), the operator

$$\delta P(k;t) = \int_k^{k+\delta k} |\phi(k';t)\rangle \langle\phi(k';t)|\, dk' \tag{10}$$

represents the projector (the differential projection operator [5][6]) onto those states contained in the interval and characterized by the values of the parameter k within the range of values δk. The action of $\delta P(k;t)$ on a wavefunction $|\psi(t)\rangle$ is defined by

$$\delta P(k;t)|\psi(t)\rangle = \int_k^{k+\delta k} C(k';t)|\phi(k';t)\rangle\, dk'. \tag{11}$$

The application of the differential projection operator $\delta P(k;t)$ causes thus the projection of the wavefunction onto the domain of states $\phi(k;t)$ which is characterized by k values within the δk interval .

In this letter, we present a straightforward, yet rigorous, proof of the exact quantum evolution for systems whose invariant has a completely continuous spectrum supposed to be non-degenerated for reasons of simplicity. Example of a particle in a time-dependent linear potential is worked out for illustration. The case of both disrete and continuous eigenvalues can be obtained by superposition. Before proceeding further, we give the statement of the exact quantum evolution.

Given a physical system with a time-dependent Hamiltonian $H(t)$, it is possible to build an invariant operator $I(t)$ verifying (1), such that its eigenvalues ε_k are purely continuous and constants

$$I(t)\left|\phi(k;t)\right\rangle = \varepsilon_k \left|\phi(k;t)\right\rangle . \tag{12}$$

Let us call $U(t)$ the evolution operator associated to the time-dependent Hamiltonian $H(t)$. The evolution of the system obeys to the Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\left|\psi(t)\right\rangle = H(t)\left|\psi(t)\right\rangle , \tag{13}$$

under these conditions it is possible to state the exact quantum evolution:

"*If the quantum system with time-dependent Hamiltonian whose invariant has a completely continuous spectrum supposed non-degenerated is initially in an eigenstate $\left|\phi(k,0)\right\rangle$ of $I(0)$ then the state of the system at any time t will remain in the subspace generated by the eigenstates $\left|\phi(k;t)\right\rangle$ of $I(t)$ pertaining to the interval $[k, k+\delta k]$*".

In others words, the exact evolution can be formally written in terms of the evolution operator as

$$\forall k, \forall t: \quad U(t)\,\delta P(k;0) = \delta P(k;t)\,U(t) . \tag{14}$$

The proof of this last equation is straightforward. One has to take the partial derivative of $\delta P(k;t) = \int\limits_k^{k+\delta k} \left|\phi(k';t)\right\rangle\left\langle\phi(k';t)\right| dk'$ with respect to the time t, taking into acount Eqs. (1) and (12), one will get then:

$$\frac{\partial \delta P(k;t)}{\partial t} + \frac{1}{i\hbar}\left[\delta P(k;t), H\right] = 0, \tag{15}$$

which has a formal solution $\delta P(k;t) = U(t)\,\delta P(k;0)\,U^{+}(t)$.

Notice that if, initially, the system is in the state $\left|\psi(k,0)\right\rangle = \left|\phi(k,0)\right\rangle$, then (14) implies that

$$\delta P(k';t)\,U(t)\left|\psi(k,0)\right\rangle = U(t)\,\delta P(k';0)\left|\psi(k,0)\right\rangle , \tag{16}$$

expanding an arbitrary state vector $\left|\psi(t)\right\rangle$ on the basis of the instantaneous quasi-eigenfunction of $I(t)$ and using (11) we obtain

$$\left|\psi(k,t)\right\rangle = \int\limits_k^{k+\delta k} C(k';t)\left|\phi(k';t)\right\rangle dk'; \qquad \forall k' \in [k, k+\delta k] , \tag{17}$$

we see that the state $\left|\psi(k,t)\right\rangle$ belongs to the subspace generated by the states $\left|\phi(k;t)\right\rangle$ pertaining to the interval $[k, k+\delta k]$.

Inserting (17) in the Schrödinger equation (13), lead to

$$\int\limits_k^{k+\delta k} i\hbar\frac{\partial}{\partial t}C(k';t)\left|\phi(k';t)\right\rangle dk' + \int\limits_k^{k+\delta k} i\hbar C(k';t)\frac{\partial}{\partial t}\left|\phi(k';t)\right\rangle dk' = \int\limits_k^{k+\delta k} C(k';t)\,H(k';t)\left|\varphi(k';t)\right\rangle dk'. \tag{18}$$

We multiply Eq. (18) by the bra of the eigendifferential (9) introduced earlier

$$\left\langle\delta\phi(\gamma;t)\right| = \int\limits_\gamma^{\gamma+\delta\gamma} \left\langle\phi(\eta;t)\right| d\eta \tag{19}$$

this yields

$$\int\limits_k^{k+\delta k} i\hbar\frac{\partial}{\partial t}C(k';t)\left|\phi(k';t)\right\rangle dk' = \int\limits_k^{k+\delta k} C(k';t)\left\langle\delta\phi(\gamma;t)\right| H(t) - i\hbar\frac{\partial}{\partial t}\left|\phi(k';t)\right\rangle dk' \tag{20}$$

Since k can sweep all the possible values and the intervals δk should be small ($\delta k \to 0$), the equality (20) between integrals implies the equality between integrands, hence

$$i\hbar \frac{\partial}{\partial t} C(k';t) = C(k';t)\left[\langle \delta\phi(k;t)| H(t) - i\hbar\frac{\partial}{\partial t}|\phi(k';t)\rangle\right];\ k' \in [k, k+\delta k]. \tag{21}$$

This equation is easily integrated and gives:

$$C(k';t) = \delta(k'-k)\exp\left[-i\int_0^t \left(\langle \delta\phi(k;t')|\frac{1}{\hbar}H(t') - \frac{\partial}{\partial t'}|\phi(k';t')\rangle\right)dt'\right];\ k' \in [k, k+\delta k], \tag{22}$$

hence

$$|\psi(k,t)\rangle = \exp\left\{\frac{i}{\hbar}\theta_k(t)\right\}|\phi(k;t)\rangle, \tag{23}$$

where $\theta_k(t)$ is the global phase given by

$$\theta_k(t) = \int_0^t \langle \delta\phi(k;t')| i\frac{\partial}{\partial t'} - \frac{1}{\hbar}H(t')|\phi(k;t')\rangle\, dt'. \tag{24}$$

This explicit formula of the phase could not be made in the Hartley-Ray approach [2] as mentioned earlier.

As the interval $[k, k+\delta k]$ is located inside of the interval $[-\infty, +\infty]$, we can write the generalized phase in the following practical form

$$\theta_k(t) = \int_0^t \int_{-\infty}^{+\infty} \langle \phi(k';t')| i\frac{\partial}{\partial t'} - \frac{1}{\hbar}H(t')|\phi(k;t')\rangle\, dt'dk', \tag{25}$$

which embodies the central result of this paper.

To illustrate this theory, let us calculate this phase for a particle moving in a time dependent linear potential

$$H(t) = \frac{1}{2m}p^2 + f(t)\,x, \tag{26}$$

where $f(t)$ is a time-dependent function. We look for the invariant of the form

$$I(t) = a(t)\,p^2 + b(t)\,p + c(t)\,x + d(t). \tag{27}$$

The invariant equation (1) is satisfied if the time-dependent coefficients are such that

$$a = a_0, \tag{28}$$

$$b = 2a_0\int_0^t f\ dt' - c_0\int_0^t \frac{1}{m}dt' + b_0, \tag{29}$$

$$c = c_0, \tag{30}$$

$$d = 2a_0\int_0^t f\ \int_0^{t'} f\ dt'dt" - c_0\int_0^t f\ \int_0^{t'} \frac{1}{m}dt'dt" + b_0\int_0^t f\ dt' + d_0, \tag{31}$$

where a_0, b_0, c_0 and d_0 are arbitrary real constants. We can choose $a_0 = 1$ and $d_0 = 0$ without loss of generalities. The eigenstates of $I(t)$ corresponding to time-independent eigenvalues k are the solutions of the equation

$$\left[-\hbar^2\frac{\partial^2}{\partial x^2} - i\hbar b\frac{\partial}{\partial x} + c_0 x + d\right]\ \phi_k(x,t) = k\phi_k(x,t). \tag{32}$$

The key point of our analysis is to perform the time-dependent unitary transformation such that

$$\Phi_k(x) = \Xi(t)\phi_k(x,t), \tag{33}$$

where a time-dependent unitary operator $\Xi(t)$ is given by

$$\Xi(t) = \exp\left(i\frac{1}{\hbar c_0}\left(\frac{b^2}{4} - d\right)p\right) \times \exp\left(i\frac{b}{2\hbar}x\right). \tag{34}$$

It can be easily shown that, under this transformation, the coordinate and momentum operators change according to

$$x \longrightarrow \Xi(t)x\Xi(t)^+ = x + \frac{1}{c_0}\left(\frac{b^2}{4} - d\right), \tag{35}$$

$$p \longrightarrow \Xi(t)p\Xi(t)^+ = p - \frac{b}{2}. \tag{36}$$

An important property of the transformation $\exp\left(-i\frac{1}{\hbar c_0}\left(\frac{b^2}{4} - d\right)p\right)$, the action of which on a wave function in the x representation reads

$$\exp\left(-i\frac{1}{\hbar c_0}\left(\frac{b^2}{4} - d\right)p\right) F(x,t) = F\left[x - \frac{1}{c_0}\left(\frac{b^2}{4} - d\right), t\right]. \tag{37}$$

Hence, the operator I changes into time-independent operator $I_0 = \Xi\ I\ \Xi^+ = p^2 + c_0 x$. In other words, the eigenvalue equation (32) for the transformed invariant operator can be simply represented in the form of Airy equation

$$\left[\frac{\partial^2}{\partial Z^2} - Z\right]\ \Phi_k(Z) = 0, \tag{38}$$

where we have introduced a new variable Z related to x through the relation $Z = \left(\frac{c_0}{\hbar^2}\right)^{\frac{1}{3}}(x - \frac{k}{c_0})$.The solution of the fundamental one dimensional ordinary second-order differential equation (38) is well-known

$$\Phi_k(x) = \frac{1}{2\pi}\left(\frac{1}{c_0\hbar^4}\right)^{\frac{1}{6}}\ Ai\left(\left(\frac{c_0}{\hbar^2}\right)^{\frac{1}{3}}\left[x - \frac{k}{c_0}\right]\right), \tag{39}$$

$Ai\left(x\right) = \int\limits_{-\infty}^{+\infty} e^{i\lambda x} e^{i\frac{\lambda^3}{3}} d\lambda$ being the integral representation of the Airy function. It is easy to verify that $\left\langle \Phi_{k'} \left| \Phi_k \right.\right\rangle = \delta\left(k - k'\right)$.

Reversing the procedure above, we can obtain

$$\phi_k\left(x,t\right) = \frac{1}{2\pi}\left(\frac{1}{c_0\hbar^4}\right)^{\frac{1}{6}} \exp\left[-i\frac{b}{2\hbar}x\right] Ai\left(\left(\frac{c_0}{\hbar^2}\right)^{\frac{1}{3}}\left[x - \frac{1}{c_0}\left(\frac{b^2}{4} + k - d\right)\right]\right). \tag{40}$$

There remains the problem of finding the phases $\theta_k(t)$ which satisfy (25). Carrying out the unitary transformation Ξ the right -hand side of Eq. (25) becomes

$$\begin{aligned}\left\langle \phi_{k'} \left| i\hbar\frac{\partial}{\partial t} - H\left(t\right)\right| \phi_k \right\rangle &= -\frac{1}{2m}\left\langle \Phi_{k'} \left| \left[I_0 + \frac{b^2}{2} - d\right] \right| \Phi_k \right\rangle \\ &= -\frac{1}{2m}\left[k + \frac{b^2}{2} - d\right]\delta\left(k - k'\right),\end{aligned} \tag{41}$$

where we have used $I_0 \left|\Phi_k\right\rangle = k\left|\Phi_k\right\rangle$ and the δ Dirac normalisation of Φ_k. Note that if $k = k'$ the latter Eq. (41) leads to an unfounded result (equal to infinity) as was mentioned earlier. Hence the phase (25) is found to be

$$\theta_k(t) - \theta_k(0) = -\frac{1}{2m}\int\limits_0^t \left[k + \frac{b^2}{2} - d\right] dt'. \tag{42}$$

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